Geostatistical Model, Covariance structure and Cokriging

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Introduction

Geostatistics and Gaussian processes

Geostatistics

- is not limited to *Gaussian processes*,
- it usually refers to the concept of *random functions,*
- it may also build on concepts from *random sets* theory.

Geostatistics

- Geostatistics:
  - is mostly known for the *kriging techniques*,
  - nowadays deals much with *geostatistical simulation.*

- *Bayesian inference* of geostatistical parameters has also become a topic of research.
- *Sequential data assimilation* is an extension of geostatistics using a mechanistic model to describe the time dynamics.

In this talk:

- we will stay with linear (Gaussian) geostatistics,
- concentrate on kriging in a multi-scale and multi-variate context.

A typical application may be:

- the response surface estimation problem
- eventually with several correlated response variables.

Statistical inference of parameters will not be discussed.

Statistics vs Machine Learning ?

Necessity of an interface meeting

Differences (subjective):

- geostatistics favours **interpretability** of the statistical model,
- machine learning stresses **prediction performance** and computational perfomance of algorithms.

Ideally both should be achieved.

Geostatistics: definition

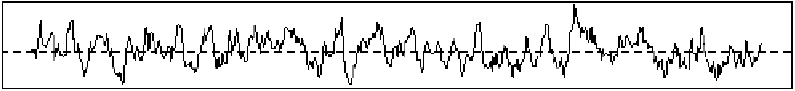
Geostatistics is an application of the theory of regionalized variables to the problem of predicting spatial phenomena.

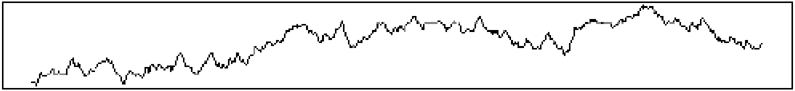
(G. MATHERON, 1970)

Usually we consider the regionalized variable $z(\mathbf{x})$ to be a realization of a random function $Z(\mathbf{x})$.

Stationarity

- For the top series:
  - we think of a (2nd order) stationary model





- For the bottom series:
  - a mean and a finite variance do not make sense,
  - rather the realization of a non-stationary process without drift.

Second-order stationary model

Mean and covariance are translation invariant

- The mean of the random function does not depend on x:

$$\mathrm{E}\Big[\, Z(\mathbf{x}) \,\Big] = m$$

- The covariance depends on length and orientation of the vector $\mathbf{h}$ linking two points $\mathbf{x}$ and $\mathbf{x}' = \mathbf{x} + \mathbf{h}$:

$$cov(Z(\mathbf{x}), Z(\mathbf{x}')) = C(\mathbf{h}) \quad = \quad \mathrm{E}\Big[\Big(Z(\mathbf{x}) - m\Big) \cdot \Big(Z(\mathbf{x}+\mathbf{h}) - m\Big) \Big]$$

Non-stationary model (without drift)

Variance of increments is translation invariant

- The mean of increments does not depend on $\mathbf{x}$ and is zero:

$$\mathrm{E}\Big[Z(\mathbf{x}+\mathbf{h})-Z(\mathbf{x})\Big]=m(\mathbf{h})=0$$

- The variance of increments depends only on $\mathbf{h}$:

$$\mathrm{var}\Big[Z(\mathbf{x}+\mathbf{h})-Z(\mathbf{x})\Big]=2\,\gamma(\mathbf{h})$$

This is called **intrinsic stationarity**.

- *Intrinsic stationarity does not imply 2nd order stationarity*.
- *2nd order stationarity implies stationary increments.*

The variogram

With intrinsic stationarity:

$$\gamma(\mathbf{h}) \quad = \quad \frac{1}{2}\,\mathrm{E}\Big[\Big(Z(\mathbf{x}+\mathbf{h}) - Z(\mathbf{x})\Big)^2\Big]$$

Properties

- zero at the origin $\quad \gamma(0) = 0$
- positive values $\quad \gamma(\mathbf{h}) \geq 0$
- even function $\quad \gamma(\mathbf{h}) = \gamma(-\mathbf{h})$

- The covariance function is bounded by the variance:
  $C(0) = \sigma^2 \geq |C(\mathbf{h})|$
  The variogram is not bounded.
- A variogram can always be constructed
  from a given covariance function: $\gamma(\mathbf{h}) = C(0) - C(\mathbf{h})$
  The converse is not true.

What is a variogram ?

- A covariance function is a **positive definite function.**

What is a variogram?

- A variogram is a **conditionnally negative definite function.** In particular:
  - any variogram matrix $\mathbf{\Gamma} = [\gamma(\mathbf{x}_\alpha - \mathbf{x}_\beta)]$ is conditionally negative semi-definite,

$$[w_\alpha]^\top \big[\gamma(\mathbf{x}_\alpha - \mathbf{x}_\beta)\big] [w_\alpha] = \mathbf{w}^\top \mathbf{\Gamma} \mathbf{w} \quad \leq \quad 0$$

for any set of weights with

$$\sum_{\alpha=0}^{n} w_\alpha = 0.$$

Ordinary kriging

Estimator: $$Z^\star(\mathbf{x}_0) = \sum_{\alpha=1}^{n} w_\alpha\, Z(\mathbf{x}_\alpha) \qquad \text{with} \sum_{\alpha=1}^{n} w_\alpha = 1$$

Solving:

$$\underset{w_1,\dots,w_n,\mu}{\arg\min} \left[\mathrm{var}\,(Z^\star(\mathbf{x}_0) - Z(\mathbf{x}_0)) - 2\mu(\sum_{\alpha=1}^{n} w_\alpha - 1) \right]$$

yields the system:

$$\begin{cases} \sum_{\beta=1}^{n} w_\beta\, \gamma(\mathbf{x}_\alpha - \mathbf{x}_\beta) + \mu & = \boxed{\gamma(\mathbf{x}_\alpha - \mathbf{x}_0)} \qquad \forall\alpha \\ \sum_{\beta=1}^{n} w_\beta & = 1 \end{cases}$$

and the kriging variance: $$\sigma_{\mathrm{K}}^2 = \mu + \sum_{\alpha=1}^{n} w_\alpha\, \gamma(\mathbf{x}_\alpha - \mathbf{x}_0)$$

Kriging the mean

Stationary model: $Z(x) = Y(x) + m$

Estimator: $$\mathrm{M}^\star = \sum_{\alpha=1}^{n} w_\alpha \, Z(\mathbf{x}_\alpha) \qquad \text{with} \sum_{\alpha=1}^{n} w_\alpha = 1$$

Solving:

$$\underset{w_1,\ldots,w_n,\mu}{\arg\min} \left[\mathrm{var}\left(\mathrm{M}^\star - m\right) - 2\mu\Big(\sum_{\alpha=1}^{n} w_\alpha - 1 \Big) \right]$$

yields the system:

$$\begin{cases} \displaystyle\sum_{\beta=1}^{n} w_\beta \, C(\mathbf{x}_\alpha - \mathbf{x}_\beta) - \mu = \boxed{0} & \forall \alpha \\ \displaystyle\sum_{\beta=1}^{n} w_\beta = 1 & \end{cases}$$

and the kriging variance: $\sigma_{\mathrm{K}}^2 = \mu$

Kriging a component

Stationary model: $Z(x) = \sum_{u=0}^{S} Y_u(x) + m \qquad (\mathrm{Y_u} \perp \mathrm{Y_v}\,\mathrm{for}\, u \neq v)$

Estimator: $\quad Y^{\star}_{u_0}(\mathbf{x}_0) = \sum_{\alpha=1}^{n} w_\alpha \, Z(\mathbf{x}_\alpha) \qquad \text{with} \sum_{\alpha=1}^{n} w_\alpha = 0$

Solving:

$$\underset{w_1,\ldots,w_n,\mu}{\arg\min} \left[\mathrm{var}\left(Y^{\star}_{u_0}(\mathbf{x}_0) - Y_{u_0}(\mathbf{x}_0) \right) - 2\mu \sum_{\alpha=1}^{n} w_\alpha \right]$$

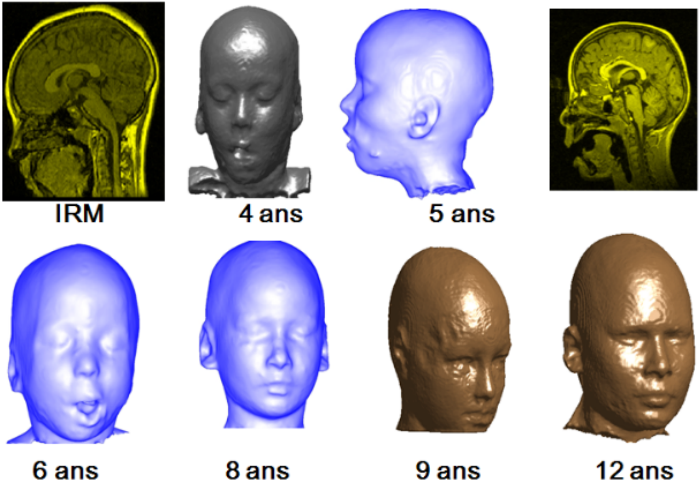
yields the system:

$$\begin{cases} \sum_{\beta=1}^{n} w_\beta \, C(\mathbf{x}_\alpha - \mathbf{x}_\beta) - \mu = \boxed{C_{u_0}(\mathbf{x}_\alpha - \mathbf{x}_0)} & \forall \alpha \\ \sum_{\beta=1}^{n} w_\beta = 0 & \end{cases}$$

Mobile phone exposure of children

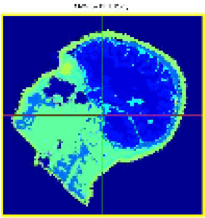
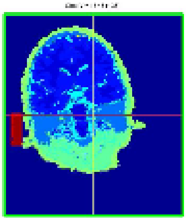
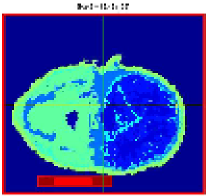
by Liudmila KUDRYAVTSEVA
http://perso.rd.francetelecom.fr/joe.wiart/

Child heads at different ages

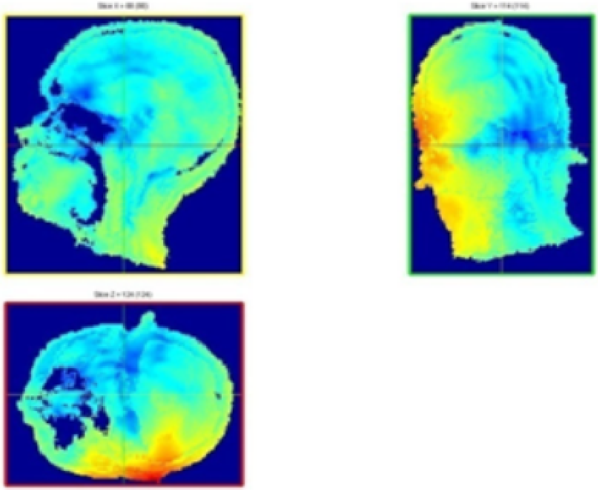


Phone position and child head

Head of 12 year old child

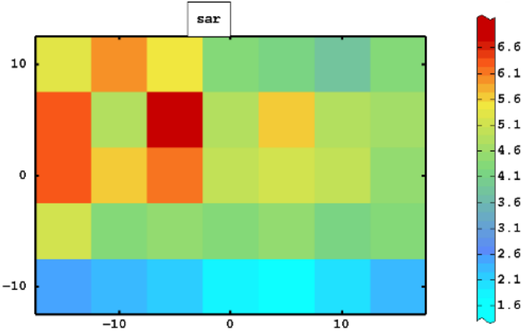
SAR exposure (simulated)



Max SAR for different positions of phone

The phone positions are characterized by two angles

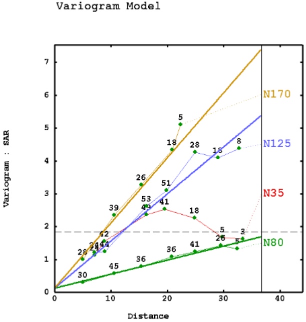
Z/X	-15	-10	-5	0	5	10	15
S4 -10	2,4601	2,2891	2,1066	1,8331	1,657	2,0705	2,2819
S1 -5	5,1367	4,3231	4,4375	4,2736	4,5223	4,1694	4,3654
S0 0	6,3054	5,6619	6,2186	5,0129	5,1247	4,977	4,4238
S2 5	6,2438	4,9029	6,8485	4,7779	5,7162	4,901	4,6314
S3 10	5,3126	5,9286	5,5342	4,3319	4,2397	3,8384	4,35



The SAR values are normalized with respect to 1 W.

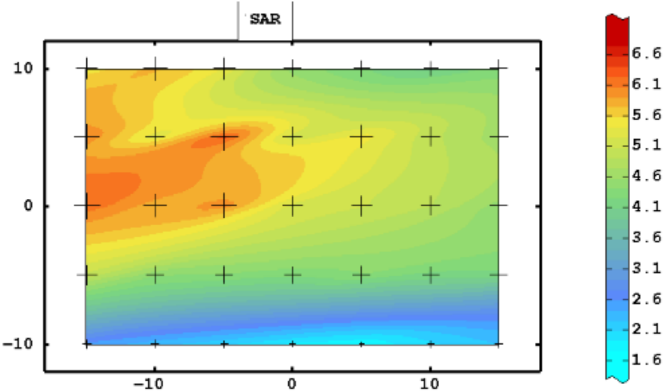
Variogram

Anisotropic linear variogram model

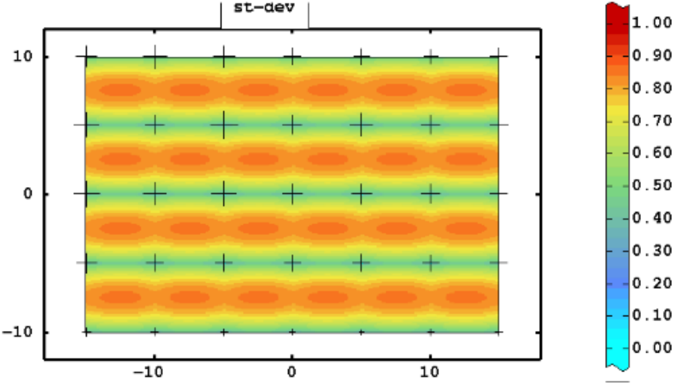



```
Isatis
DIR/donnees_completes
- Variable #1 : SAR
Experimental Variogram : in 4 direction(s)
D1   : N35
       Angular tolerance =  22.50
       Lag =  5.00m, Count = 8 lags, Tolerance = 70.00%
D2   : N80
       Angular tolerance =  22.50
       Lag =  5.00m, Count = 8 lags, Tolerance = 70.00%
D3   : N125
       Angular tolerance =  22.50
       Lag =  5.00m, Count = 8 lags, Tolerance = 70.00%
D4   : N170
       Angular tolerance =  22.50
       Lag =  5.00m, Count = 8 lags, Tolerance = 70.00%
Model : 2 basic structure(s)
S1   - Nugget effect, Sill =     0.1299
S2   - Power - Scale = 28.21m - Exp. = 1.00, Sill =      5.591
       Directional Scales = (    130.98m,     28.21m)
       Rotation = Azimuth=80.00 (Geologist)
```

Max SAR kriged map

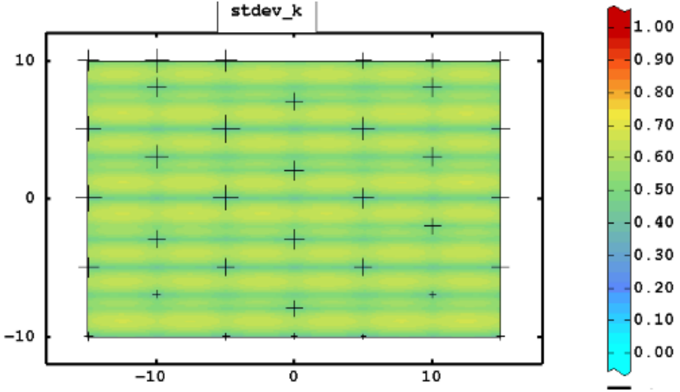


Kriging standard deviations



Kriging standard deviations

Different sample design

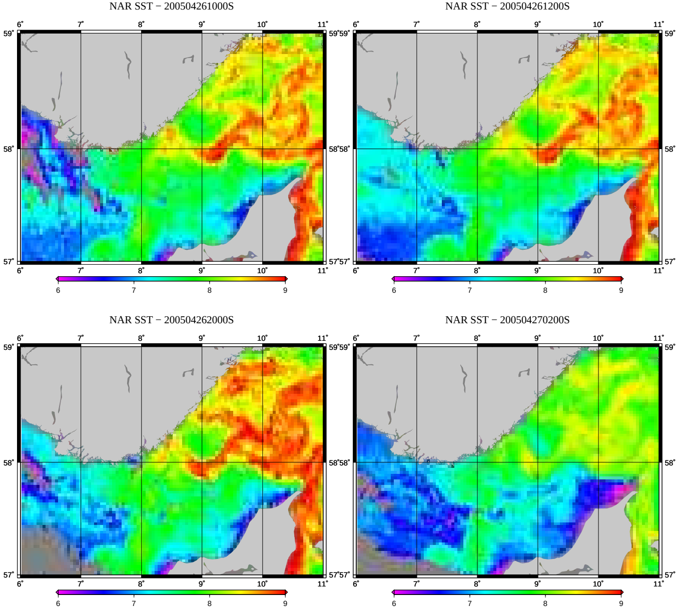


Geostatistical filtering:

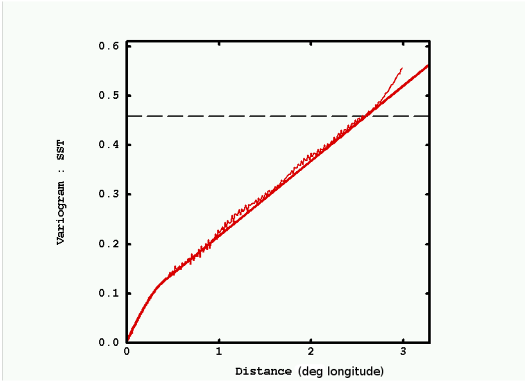
Skagerrak SST

NAR16 images on 26-27 april 2005

Sea-surface temperature (SST)



Nested variogram model



Nested scales modeled by sum of different variograms:

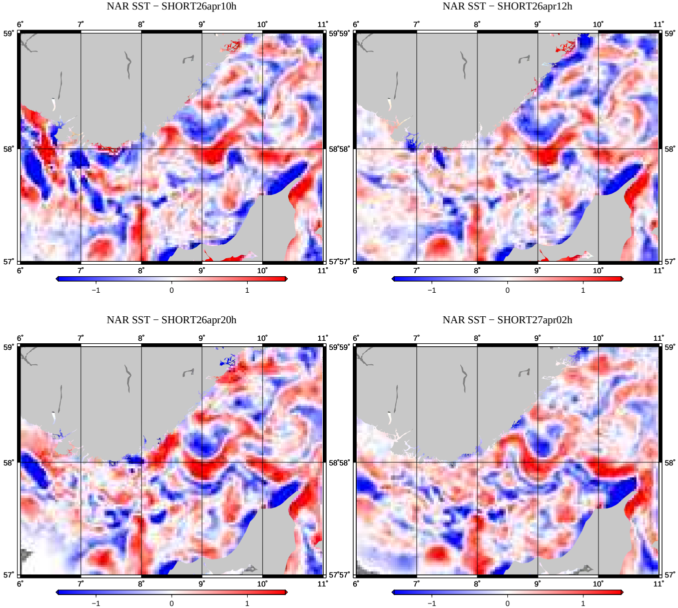
micro-scale nugget-effect of .005

small scale spherical model (range .4 deg longitude, sill .06)

large scale linear model

Geostatistical filtering

Small-scale variability of NAR16 images



Geostatistical Model

Linear model of coregionalization

The linear model of coregionalization (LMC) combines:

- a linear model for different scales of the spatial variation,
- a linear model for components of the multivariate variation.

Two linear models

- **Linear Model of Regionalization:**

$$\boxed{Z(\mathbf{x}) = \sum_{u=0}^{S} Y_u(\mathbf{x})}$$

  - $\mathrm{E}\Big[\, Y_u(\mathbf{x}+\mathbf{h}) - Y_u(\mathbf{x}) \,\Big] = 0$
  - $\mathrm{E}\Big[\Big(Y_u(\mathbf{x}+\mathbf{h}) - Y_u(\mathbf{x}) \Big) \cdot \Big(Y_v(\mathbf{x}+\mathbf{h}) - Y_v(\mathbf{x}) \Big) \Big] = g_u(\mathbf{h})\, \delta_{uv}$

- **Linear Model of PCA:**

$$\boxed{Z_i = \sum_{p=1}^{N} a_{ip}\, Y_p}$$

  - $\mathrm{E}\Big[\, Y_p \,\Big] = 0$
  - $\mathrm{cov}\Big(Y_p, Y_q \Big) = 0 \quad$ for $p \neq q$

Linear Model of Coregionalization

Spatial and multivariate representation of $Z_i(\mathbf{x})$ using uncorrelated factors $Y_u^p(\mathbf{x})$ with coefficients a_{ip}^u:

$$\boxed{Z_i(\mathbf{x}) = \sum_{u=0}^{S} \sum_{p=1}^{N} a_{ip}^u \, Y_u^p(\mathbf{x})}$$

Given u, all factors $Y_u^p(\mathbf{x})$ have the same variogram $g_u(\mathbf{h})$.

This implies a **multivariate nested variogram**:

$$\mathbf{\Gamma}(\mathbf{h}) = \sum_{u=0}^{S} \mathbf{B}_u \, g_u(\mathbf{h})$$

Coregionalization matrices

The coregionalization matrices $\mathbf{B}_u$ characterize
the correlation between the variables Z_i
at different spatial scales.

In practice:

1. A multivariate nested variogram model is fitted.
2. Each matrix is then decomposed using a PCA:

$$\mathbf{B}_u = \left[b_{ij}^u \right] = \left[\sum_{p=1}^{N} a_{ip}^u \, a_{jp}^u \right]$$

yielding the coefficients of the LMC.

LMC: intrinsic correlation

When all coregionalization matrices are **proportional** to a matrix **B**:

$$\mathbf{B}_u = a_u\,\mathbf{B}$$

we have an intrinsically correlated LMC:

$$\boldsymbol{\Gamma}(\mathbf{h}) = \mathbf{B}\sum_{u=0}^{S} a_u\, g_u(\mathbf{h}) = \mathbf{B}\,\gamma(\mathbf{h})$$

In practice, with intrinsic correlation, the eigenanalysis of the different $\mathbf{B}_u$ *will yield:*

- different sets of eigenvalues,
- but identical sets of eigenvectors.

Regionalized Multivariate Data Analysis

- **With intrinsic correlation:**

The factors are autokrigeable,
i.e. the factors can be computed
from a classical MDA on
the variance-covariance matrix $\mathbf{V} \cong \mathbf{B}$
and are **kriged** subsequently.

- **With spatial-scale dependent correlation:**

The factors are defined on the basis of
the coregionalization matrices $\mathbf{B}_u$
and are **cokriged** subsequently.

Need for a regionalized multivariate data analysis!

Regionalized PCA ?

$$\begin{tikzcd}
\boxed{\text{Variables } Z_i(\mathbf{x})} \arrow[d] & \\
\boxed{\text{Intrinsic Correlation ?}} \arrow[r, "\text{no}"] \arrow[d, "\text{yes}"] & \boxed{\gamma_{ij}(\mathbf{h}) = \sum_u \mathbf{B}_u\, g_u(\mathbf{h})} \arrow[d] \\
\boxed{\text{PCA on } \mathbf{B}} \arrow[d] & \boxed{\text{PCA on } \mathbf{B}_u} \arrow[d] \\
\boxed{\text{Transform into } \mathbf{Y}} \arrow[d] & \boxed{\text{Cokrige } Y^\star_{u_0 p_0}(\mathbf{x})} \arrow[d] \\
\boxed{\text{Krige } Y^\star_{p_0}(\mathbf{x})} \arrow[r] & \boxed{\text{Map of PC}}
\end{tikzcd}$$

Geostatistical filtering: Golfe du Lion SST

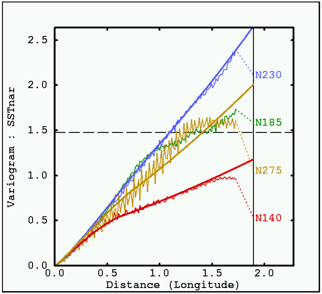
Modeling of spatial variability

as the sum of a small-scale and a large-scale process

SST on 7 june 2005

The variogram of the Nar16 image is fitted with a short- and a long-range structure (with geometrical anisotropy).

Variogram of SST



The small-scale components

- of the NAR16 image

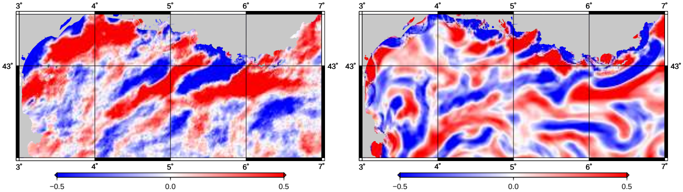
and

- of corresponding MARS ocean-model output

are extracted by geostatistical filtering.

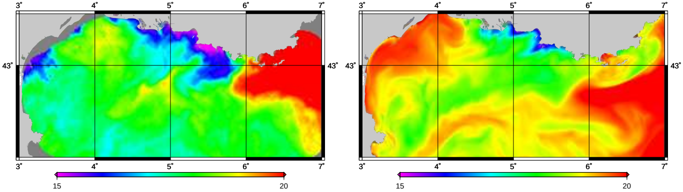
Geostatistical filtering

Small scale (top) and large scale (bottom) features



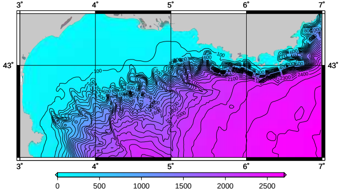
NAR16 image

MARS model output

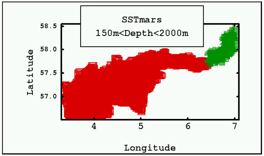


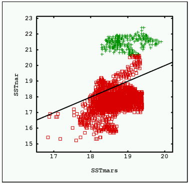
Zoom into NE corner

Bathymetry

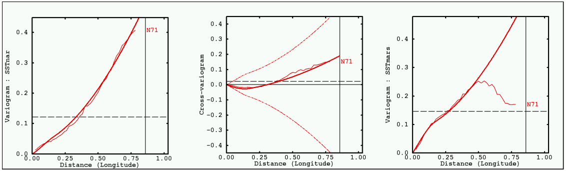


Depth selection, scatter diagram



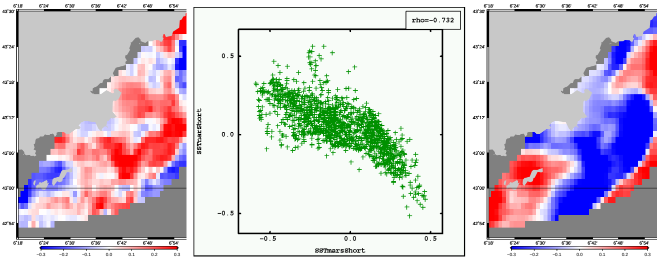


Direct and cross variograms in NE corner



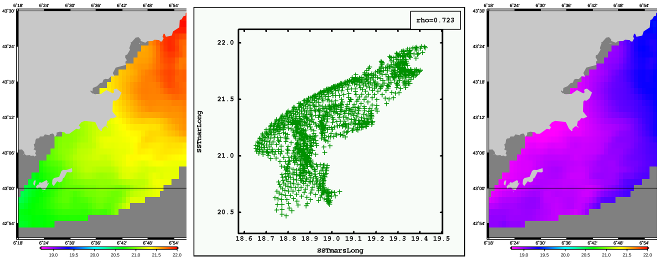
Cokriging in NE corner

Small scale (top) and large scale (bottom) components



NAR16 image

MARS model output



Interpretation

To correct for these discrepancies between remotely sensed SST and that provided by the MARS ocean model, the latter was thoroughly revised in order better reproduce the path of the Ligurian current.

Covariance structure

Intrinsic Correlation: Variogram Model

A simple model for the matrix $\mathbf{\Gamma}(\mathbf{h})$ of direct and cross variograms $\gamma_{ij}(\mathbf{h})$ is:

$$\mathbf{\Gamma}(\mathbf{h}) = \Big[\gamma_{ij}(\mathbf{h})\Big] = \mathbf{B}\,\gamma(\mathbf{h})$$

where $\mathbf{B}$ is a positive semi-definite matrix.

In this model all variograms are proportional to a basic variogram $\gamma(\mathbf{h})$:

$$\gamma_{ij}(\mathbf{h}) = b_{ij}\,\gamma(\mathbf{h})$$

Codispersion Coefficients

- A coregionalization is **intrinsically correlated** when the codispersion coefficients:

$$\mathrm{cc}_{ij}(\mathbf{h}) = \frac{\gamma_{ij}(\mathbf{h})}{\sqrt{\gamma_{ii}(\mathbf{h})\,\gamma_{jj}(\mathbf{h})}}$$

are constant, i.e. do not depend on spatial scale.

- With the **intrinsic correlation model**:

$$\mathrm{cc}_{ij}(\mathbf{h}) = \frac{b_{ij}\ \gamma(\mathbf{h})}{\sqrt{b_{ii}\,b_{jj}}\,\gamma(\mathbf{h})} = r_{ij}$$

the correlation r_{ij} between variables is not a function of $\mathbf{h}$.

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  the correlation r_{ij} between variables is not a function of **h**.

Intrinsic Correlation: Covariance Model

- For a covariance function matrix the model becomes:

$$\mathbf{C}(\mathbf{h}) = \mathbf{V}\,\rho(\mathbf{h})$$

  where
  - $\mathbf{V} = \left[\sigma_{ij}\right]$ is the variance-covariance matrix,
  - $\rho(\mathbf{h})$ is an autocorrelation function.

- The correlations between variables do not depend on the spatial scale **h**, hence the adjective ***intrinsic***.
- In the intrinsic correlation model the multi-variate variability is **separable** from the spatial variation.

A Test for Intrinsic Correlation

1. Compute principal components for the variable set.
2. Compute the cross-variograms between principal components.

- In case of intrinsic correlation, the cross-variograms between principal components are all zero.

A Test for Intrinsic Correlation

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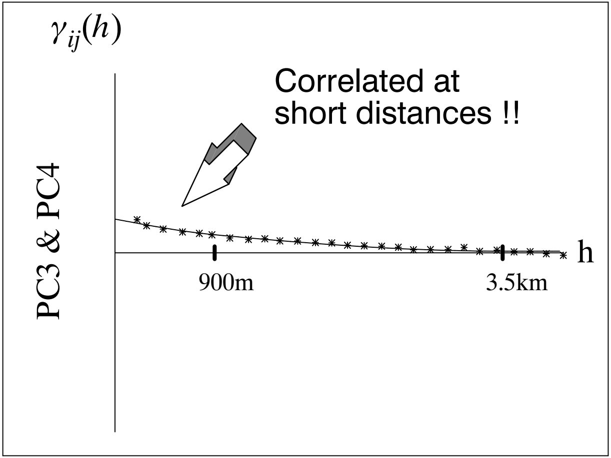
Cross variogram: two principal components



$\Longrightarrow$ The intrinsic correlation model is not adequate!

Cokriging

Multivariate Kriging

Kriging is optimal linear unbiased prediction applied to random functions in space or time with the particular requirement that their covariance structure is known.
$\longrightarrow$ Multivariate case: co-kriging

Covariance structure: covariance functions (or variograms, generalized covariances) for a set of variables.

Ordinary cokriging

Estimator: $Z^{\star}_{i_0,\mathrm{OK}}(\mathbf{x}_0) \;=\; \sum_{i=1}^{N}\sum_{\alpha=1}^{n_i} w^i_\alpha\, Z_i(\mathbf{x}_\alpha)$

- constrained weights: $\sum_{\alpha} w^i_\alpha = \delta_{i,i_0}$
- valid for variograms,
- nonstationary phenomenon without drift.

Data configuration & Cokriging neighborhood

- Data configuration:
  sites of different types of measurements
  in a spatial/temporal domain.

  Are sites shared by different measurement types — or not?

- Neighborhood:
  a subset of data used in cokriging.

  How should the cokriging neighborhood be defined?

  What are the links with the covariance structure?

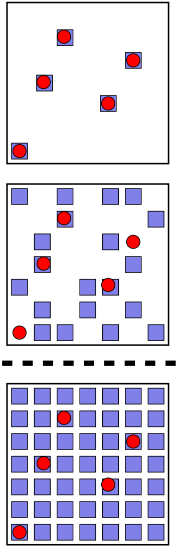
Configurations: Iso- and Heterotopic Data

● primary data ■ secondary data

Isotopic data

Sample sites

are shared



Heterotopic data

Sample sites

may be different

Dense auxiliary data

Secondary data

covers whole domain

Configuration: isotopic data

Auto-krigeability

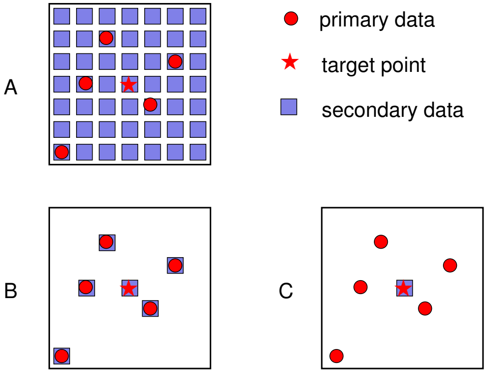
A random function $Z_1(\mathbf{x})$ is **auto-krigeable** (self-krigeable), if the cross-variograms of that variable with the other variables are all proportional to the direct variogram of $Z_1(\mathbf{x})$:

$$\gamma_{1j}(\mathbf{h}) = a_{1j}\,\gamma_{11}(\mathbf{h}) \qquad \text{for} \quad j = 2, \ldots, N$$

- Isotopic data: **auto-krigeability** means that the cokriging boils down to the corresponding kriging.
- If all variables are auto-krigeable, the set of variables is **intrinsically correlated**, i.e. the multivariate variation is separable from the spatial variation.

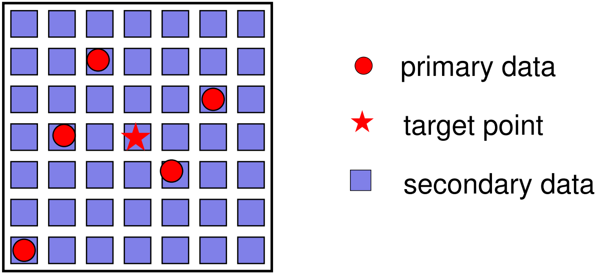
Configuration: dense auxiliary data

3 cokriging neighborhoods



A: neighborhood using all data
B: multi-collocated neighborhood
C: collocated neighborhood

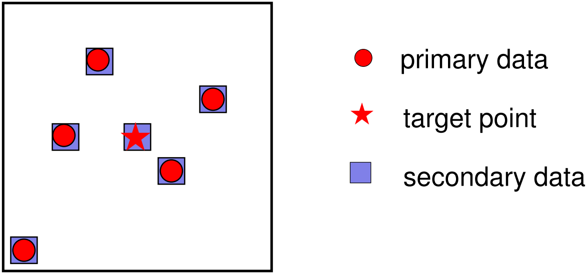
Neighborhood: all data



Very dense auxiliary data (e.g. remote sensing): *a priori* large cokriging system, potential numerical instabilities. Ways out:

- moving neighborhood,
- multi-collocated neighborhood,
- sparser cokriging matrix: covariance tapering.

Neighborhood: multi-collocated



- Multi-collocated cokriging equivalent to cokriging with all data when there is proportionality in the cross-covariance model,
- for all forms of cokriging: simple, ordinary, universal

Neighborhood: multi-collocated

Bivariate example: proportionality in the covariance model

Cokriging with all data is equivalent to cokriging with a multi-collocated neighborhood for a model with a covariance structure is of the type:

$$\begin{aligned} C_{11}(\mathbf{h}) &= p^2\, C(\mathbf{h}) + C_1(\mathbf{h}) \\ C_{22}(\mathbf{h}) &= C(\mathbf{h}) \\ C_{12}(\mathbf{h}) &= p\, C(\mathbf{h}) \end{aligned}$$

where p is a proportionality coefficient.

RIVOIRARD (2004) studies various examples of this kind, examining bivariate and multi-variate coregionalization models in connection with different data configurations and neighborhoods, among them the **dislocated neighbohood**.

Acknowledgements

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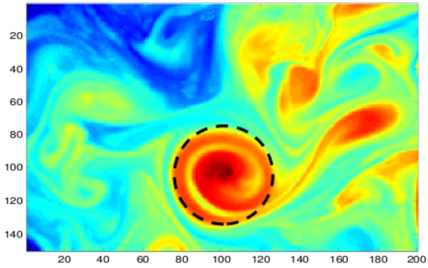
Appendix

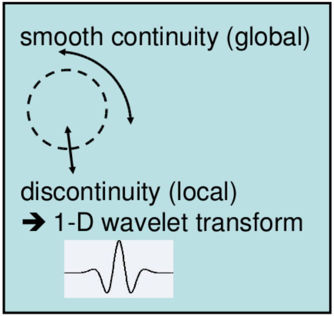
Eddie tracking with circlets

by Hervé CHAURIS www.geophy.ensmp.fr

Detection of circular structures

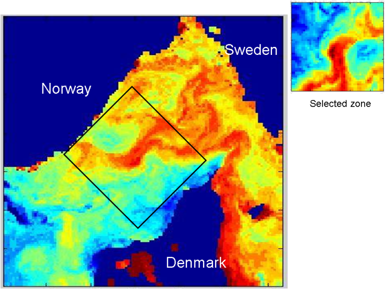
Taking account of the band limited aspect of the data:



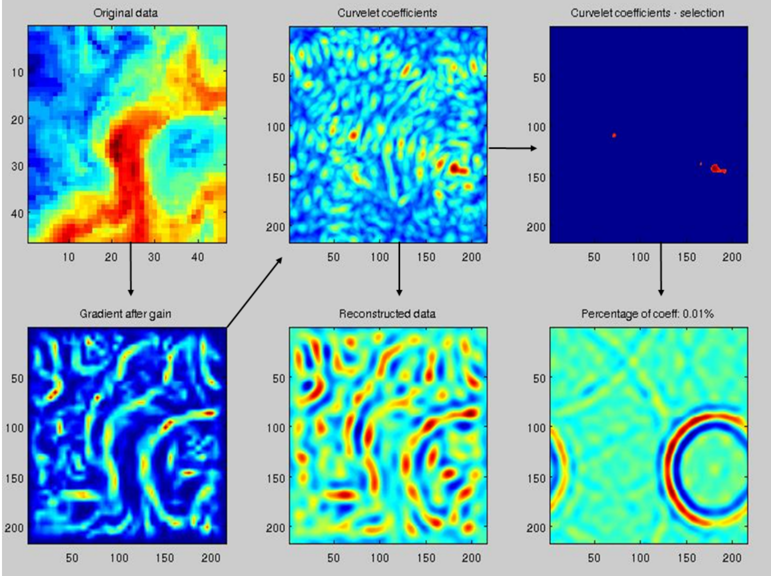


Circlets applied to Skagerrak

- Preprocessing (despiking, transfer on regular grid); image gradient;
- circlet decomposition; coefficient thresholding;
- Image reconstruction.

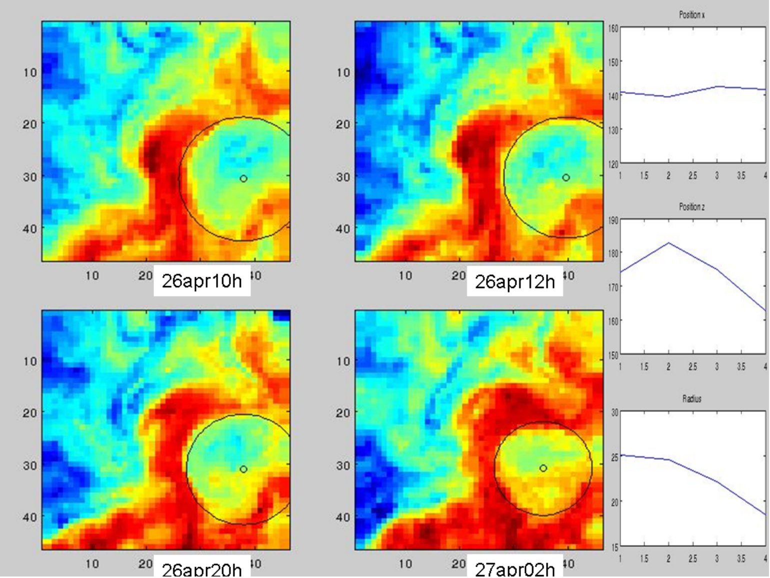


Methodology



Circlets applied to Skagerrak

Tracking the position and diameter of an eddy-like structure



Potential of circlets

- Preprocessing can be done by *geostatistical filtering*
- Simple and fast circlet transform
  (CPU cost of a few 2-D FFTs)
- Deal with edge effects
- How to integrate eddie tracking into a data assimilation procedure?